Narrowing the search for new materials

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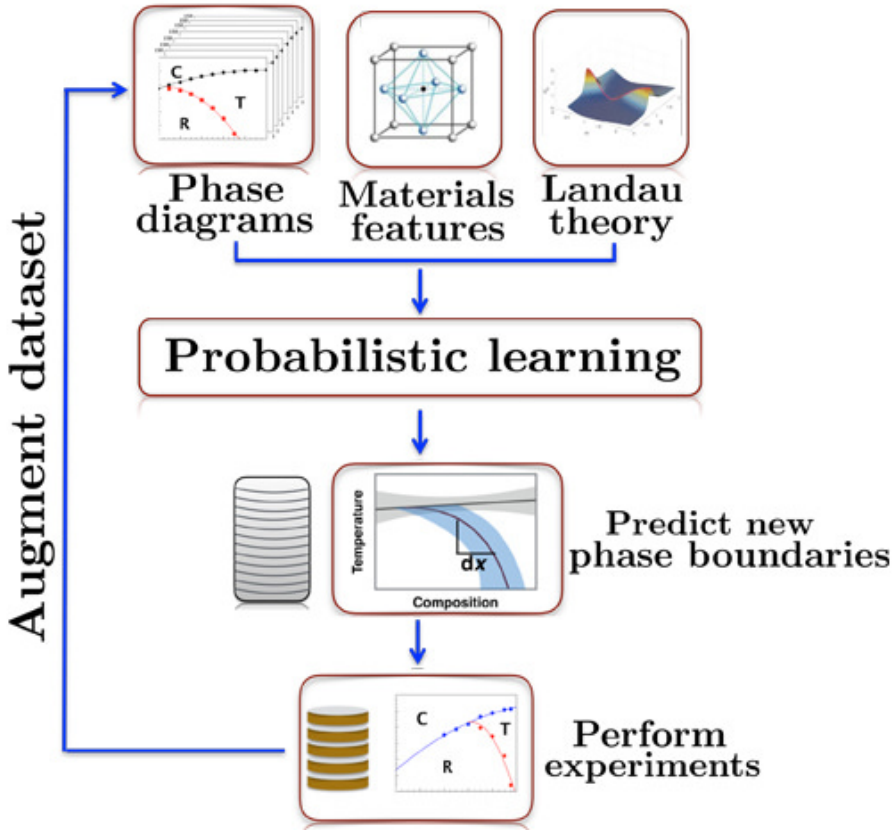

Data science guides discovery of new lead-free piezoelectric materials

Piezoelectric compounds are widely used in converting mechanical pressure into electrical energy. One of the most widely used examples is the starter on gas stoves and gas barbecue grills. Some of these piezoelectrics are made up of hazard elements such as lead. Efforts to accelerate the discovery of new piezoelectric materials are an emerging theme as well as an outstanding challenge in materials science.

A new national initiative has so far largely focused on generating and screening databases of information derived from computer codes or using historic data to make predictions, much like predicting the stock market based on past performance. In materials science there exists a substantial body of knowledge in the form of physical theories and models, which could be used to make more robust predictions than from data alone. These theories and models become especially valuable when the available data are limited or small. “This (small data problem) is often an underappreciated factor

in materials informatics” says Turab Lookman, Physicist and Materials Scientist at Los Alamos National Lab (LANL). His team has been working on developing novel data science methods to accelerate the search for new materials. Materials science typically gives rise to relatively small amounts of data (10-100 well characterized samples) as experiments are limited by the availability of new materials. Increasing the usefulness of this data to make predictions is an outstanding challenge in the field.

Los Alamos National Laboratory researchers, which included post-doctoral fellows D. Xue and P.V. Balachandran, with collaborators (E. Dougherty and his group) at the Center for Genomic Studies at Texas A&M University, have now combined data analytics and materials knowledge in the form of theory to guide experiments in the design of novel lead-free piezoelectrics. In a recently published paper in the *Proceedings of National Academy of Sciences*, the researchers showed how relatively small amounts of input data from known measurements of complex compounds can lead to the predictions of new lead-free piezoelectrics with targeted response.

Using an approach developed to genetically screen cancer patients for certain drugs, the team has developed an approach to integrate prior knowledge about the behavior of piezoelectrics with observed data. This has never been explored for accelerating the search for new materials. A phase diagram that contains the results of up to 10 different compositions is combined with up to 1200 others diagrams to predict the physical character. As you already know, trying to make measurements on every one of those proposed options is totally unrealistic. The researchers designed, synthesized, and tested a new compound that is a lead-free composition. In addition to the strain of a dedicated timeline to this project, the selected compound is relatively insensitive to changes in temperature in contrast to the best compound available to date in that class.

Even with small or limited experimental data and complex theoretical relationships among material characteristics, probabilistic approaches offer the means to make robust predictions. These approaches point to targeted outcomes that can be achieved in as few experiments as possible.